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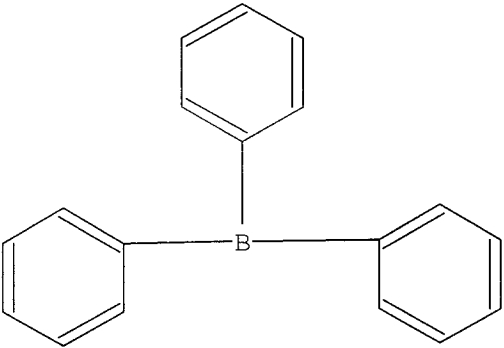
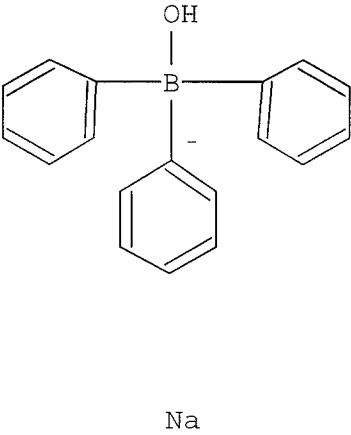
OVERALL SUMMARY FOR TRIPHENYLBORON CATEGORY

Summary

Identification of a structure based category

The triphenylboron category is composed of triphenylborane (TPB) and triphenylboron compound with sodium hydroxide (TPB-NaOH). TPB is a monofunctional Lewis acid. For shipping purposes, TPB is provided as a sodium hydroxide adduct. TPB-NaOH is produced at the plant as an approximately 8% aqueous solution containing additional free sodium hydroxide. The TPB-NaOH will dissociate into TPB and NaOH. This dissociation requires pH <7. Structures of these substances are presented below.

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<u>Chemical Name</u>	<u>CAS Registry Number</u>	<u>Structure</u>
Triphenylborane	960-71-4	
Triphenylboron compd. with sodium hydroxide	12113-07-4	

Scientific literature was searched and summarized. Data were identified for materials in the category (Table 1). Each study on category materials was evaluated for adequacy. Robust summaries were developed for each study addressing specific SIDS endpoints. Summaries were also developed for studies either considered not adequate but provided information of relevance for hazard identification and evaluation, or covered non-SIDS endpoints (Appendices A-B).

Table 1: Matrix of Available and Adequate Data for Triphenylborane Category

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Melting Point	√	√
Boiling Point	√	√
Vapor Pressure	√	√
Partition Coefficient (log Kow)	√	√
Water Solubility	√	√
Photodegradation	√	√
Stability in Water	√	√
Transport (Fugacity)	√	√
Biodegradation	√	√
Acute Toxicity to Fish	-	-
Acute Toxicity to Invertebrates	√	-
Acute Toxicity to Aquatic Plants	-	-
Acute Toxicity	√	√
Repeated Dose Toxicity	-	-
Developmental Toxicity	-	-
Reproductive Toxicity	-	-
Genetic Toxicity Bacterial Gene Mutations	√	√
Genetic Toxicity Mammalian Cell Gene Mutations	-	√
Genetic Toxicity Chromosomal Aberrations	-	-

Evaluation of Data Matrix Patterns

The available adequate data were broken out by discipline (physical chemical, environmental fate, ecotoxicology, and mammalian toxicology). Comparisons of the data were conducted to determine if additional testing is needed to complete the data set for the category.

Table 2: Physical and Chemical Characteristics

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Physical Appearance	White crystalline solid	Solid
Molecular Weight	241.8	281.8
Water Solubility	9.895×10^{-2} mg/L	2.882 mg/L
Melting Point	136°C	> 300°C
Boiling Point	347°C	644.67°C
Vapor Pressure	1.19×10^{-5} mm Hg	8.52×10^{-18} mm Hg
Density	1.1 g/cm ³	1.35 g/cm ³
Partition Coefficient (log Kow)	5.52	4.37

Environmental fate data is listed in Table 3. Triphenylborane (TPB) is reported to be unstable in water and hydrolyzes to form mixtures of phenylboric oxide and phenylboronic acid (Brown, 1957). As a product of commerce TBP(NaOH) is typically an aqueous, strongly alkaline, 8-10% solution of TBP(NaOH). Loss of the OH⁻ complex at near neutral pH results in the formation of the highly insoluble TPB, which as noted above is hydrolytically unstable in water. However, demonstration of a rate and end products for TPB hydrolysis would be most useful. Therefore, a hydrolysis study following OECD Guideline 111 is recommended for triphenylborane. The phenylboron products expected from aqueous hydrolysis of TBP are both estimated to have log Kow values ≤ 2 and a biodegradation half-life in water of approximately 15 days (Ultimate Survey Model: WEEKS) (EPIWIN v.3.11). Therefore, the TBP hydrolysis products, phenylboric oxide and phenylboronic acid, are not expected to be substantially persistent or bioaccumulative. Vapor phase TPB and TPB(NaOH) are estimated to have a half-life of 65.8 and 64.3 hours, respectively, in air (EPIWIN 3.11 AOP Program v.1.9). Moisture may shorten the half-life in air. However, with vapor pressures $< 10^{-4}$ mm Hg, most atmospheric material for this category is expected to be adsorbed to particles. Emission to dry soil may also result in a moderate soil half-life in the absence of moisture input, because the parent compound will stick strongly to soil organic matter (TPB: log Koc estimates of 1.36×10^5 and 4.45×10^5 , EPIWIN 3.11 Level III Fugacity Model and EPIWIN 3.11 PCKOC Program, v.1.66, respectively), (TPB(NaOH): log Koc estimates of 6.96×10^5 and 9.61×10^3 , EPIWIN 3.11 Level III Fugacity Model and EPIWIN 3.11 PCKOC Program, v. 1.66, respectively).

Table 3: Environmental Fate

	Triphenylborane			Triphenylboron compd. with sodium hydroxide		
Bioaccumulation*	BCF = 3558			BCF = 2727		
Biodegradation*	Weeks to months, 2.73			Weeks to months, 2.64		
Fugacity* (Equal emissions to Air, Water and Soil)	Compartment	Distribution %	½ life, hours	Compartment	Distribution %	½ life, hours
	Air	0.94	65.8	Air	0.0024	64.3
	Water	6.74	900	Water	10.3	900
	Soil	47.6	1800	Soil	83.9	1800
	Sediment	44.8	8100	Sediment	5.75	8100
* Modeled data.						

Available aquatic toxicity data are presented in Table 4. Triphenylborane was extremely toxic to *Daphnia* with a 48-hour EC₅₀ of 0.002 mg/L. Since ECOSAR cannot be used to predict toxicity of boron chemicals, and no data are available, aquatic toxicity tests on fish and algae with triphenylborane, generally following OECD guidelines 203 and 201, respectively, are recommended.

Table 4: Ecotoxicity

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Toxicity to Fish	No Data	No Data
Toxicity to Invertebrates (48-hour EC₅₀)	0.002 mg/L	No Data
Toxicity to Algae	No Data	No Data

In mammalian species the oral LD₅₀ in rats for triphenylborane and triphenylboron compd. with sodium hydroxide are 196 and 1236 mg/kg, respectively. The oral ALD (approximate lethal dose) for triphenylborane (10% active ingredient) was 2250 mg/kg and for triphenylborane compd. with sodium hydroxide (purity not reported) was 200 mg/kg. The four-hour inhalation LC₅₀ for triphenylborane is 0.073 mg/L. Triphenylborane and triphenylboron compd. with sodium hydroxide were both severe skin and eye irritants when tested in rabbits. Triphenylborane did not produce skin sensitization in guinea pigs.

Table 5: Acute Mammalian Toxicity

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Oral LD₅₀ (rat)	196 mg/kg ALD = 2250 mg/kg	1236 mg/kg ALD = 200 mg/kg
Inhalation ALC (4-hour; rat)	0.073 mg/L	No Data
Dermal LD₅₀ (rabbit)	No Data	No Data
Dermal Irritation	Corrosive (rabbits)	Severe (rabbits)
Eye Irritation	Severe	Corrosive
Dermal Sensitization	Not a sensitizer	No Data

No information regarding repeated dose, developmental, or reproductive toxicity was found. Therefore, a combined repeated dose toxicity study with the reproduction/developmental toxicity screening test (OECD Guideline 422) with triphenylborane is recommended.

Table 6: Repeated Dose, Developmental, and Reproductive Toxicity

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Repeated Dose Toxicity (NOAEL)	No Data	No Data
Developmental Toxicity	No Data	No Data
Reproductive Toxicity	No Data	No Data

Genetic toxicity data are similar between the two test substances, supporting a category approach (Table 7). Triphenylborane and triphenylboron compd. with sodium hydroxide do not induce mutations in bacteria. Additionally, triphenylboron compd. with sodium hydroxide was negative in an *in vitro* mammalian cell gene mutation study with Chinese hamster ovary cells. Since no data are available for clastogenicity, an *in vitro* clastogenicity study with triphenylborane, generally following OECD Guideline 473 is recommended.

Table 7: Genetic Toxicity

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Mutagenic	Negative	Negative
Clastogenic	No Data	No Data

Missing data elements for triphenylborane and triphenylboron compd. with sodium hydroxide, as well as the test plan are listed in Table 8.

Table 8: Proposed Test Plan for Triphenylboron Category

	Triphenylborane	Triphenylboron compd. with sodium hydroxide
Hydrolysis	Y	N ²
Toxicity to Fish	Y	N ²
Toxicity to Invertebrates	N ¹	N ²
Toxicity to Algae	Y	N ²
Combined Repeated Dose Study and Developmental/Reproductive Toxicity Screen	Y	N ³
Genetic Toxicity Chromosomal Aberrations	Y	N ³
¹ = Data available. ² = No testing will be performed since at high dilution, the likely environmental case, the hydroxide compound will decompose to triphenylborane (the relevant compound) at neutral pH. ³ = Evaluation of the test substance will be considered based upon the results obtained from the study performed with triphenylborane.		

Exposure Assessment

Triphenylborane (TPB) is manufactured at one DuPont facility. TPB is not currently sold to customers for commercial applications. For shipping purposes, TPB is supplied as a stable, easily transported aqueous caustic adduct (TPB sodium hydroxide adduct). TPB(NaOH) has not been sold to any customers for commercial applications, but several samples for R&D have been sent to potential customers. Potential applications include olefin polymerization, agrichemicals, fuel additives, metal scavenging, and flame retardants.

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The site can have 2000 personnel working (construction, contractor, and plant employees). The areas where the substance is manufactured will have 4 operators during normal operations and 14 to 32 people during a shutdown or major construction activity. The site has effective safety, health, and environmental practices and procedures, in addition to engineering controls, environmental controls, and personal protective equipment to control exposure. Adequate safety equipment, such as safety showers, eyewash fountains, and washing facilities, are available in the event of an occupational exposure.

Individuals handling TPB(NaOH) should wear safety glasses and impervious clothing, such as gloves, apron, boots, or whole bodysuit made of NBR or Neoprene, as appropriate. When the possibility exists for eye and face contact due to splashing or spraying of material, individuals should wear coverall chemical splash goggles and face shield. NIOSH approved respiratory protection should be worn as appropriate.

DuPont practices Responsible Care and assesses the ability of potential customers to safely handle TPB(NaOH) prior to commencing a commercial relationship. The Product Stewardship System works with customers to understand their applications and any issues associated with PPE (personal protective equipment), safety equipment (safety showers, eyewash stations, ventilation needs, etc.), storage concerns, disposal requirements and MSDS questions. The procedure for isolating pure TPB from the adduct solution is available to any potential customers and is accessible through the DuPont website.

No occupational exposure limits have been established. Air monitoring has not been conducted on TPB.

References for Summary:

Brown, H. C. (1957). J Amer. Chem. Soc., 79: 2303.